

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 368 °C

Global applicability domain: Inside

Local applicability domain index: 3.27e-01

Confidence level: 4.70e-01

Nearest Neighbors from the Training Set

Image not found

Dehydrothio-4-toluidine

Measured: 434

Predicted: 377

Image not found

4,4'-Methylenebis(N,N-dimethylaniline)

Measured: 390

Predicted: 349

Image not found

1,3-Dimethyl-1,3-diphenylurea

Measured: 350

Predicted: 338

Image not found

Imazalil

Measured: 347

Predicted: 338

Image not found

3,5-Diphenyl-1,2,4-oxadiazole

Measured: 290

Predicted: 317